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The role of hydrogen bonds and solvent effects on mechanical behavior of mortar coatings applied on the facades of structural masonry buildings

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Abstract: Mortar coatings applied on the facades of structural masonry buildings play an important role in the performance of vertical fences, and contribute to the waterproofing and protection of the external agents[1,2]. Routinely, the plastering mortar is employed for this purpose. It is also often employed a layer of roughcast mortar on the structural masonry before the use of the plastering mortar. In this sense, the main goal of our study was evaluated the role of the hydrogen bonds and the effect of the water as solvent to the mechanical behavior, experimentally measured, of the two strategies to apply the layer of plastering mortar on the structural masonry buildings: (i) with, and (ii) without an addition of the roughcast layer. The theoretical/computational methodology was the use of PM7 semiempirical method[3], which is available at quantum chemical software MOPAC 2016[4]. We considered the PM7 values of enthalpy of reaction, $\Delta_r H$, calculated both in the gas phase, and water solvent phase. The water solvent effects on the $\Delta_r H$ property were calculated by the COSMO model[5]. The mechanical behavior experiments were based on tensile strength tests of two walls, each one with the mortar coatings proposed in this work. Both walls evaluated in this study were performed by using concrete blocks with compressive strength of 4 MPa. Experimental results indicate that in the two cases studied, the tensile strength tests were 0.56 MPa for the case with roughcast layer, and 0.57 MPa for case without roughcast layer, i. e., the roughcast layer, seemingly, not affect the tensile strength of the material. The mechanical behavior verified can be associated with the hydrogen bonds between components of the two types of mortar employed: calcium hydroxide and silicon dioxide. Our PM7 results indicating that energy of hydrogen bonds between $Ca(HO)_2$ and water are more pronounced than the energy of hydrogen bonds between the SiO_2 and water. On average, the $\Delta_r H$ PM7 value, in the gas phase, for the possibilities of hydrogen bonded complexes [(calcium hydroxide)---$(H_2O)_n$], n=1 or 2, is -31 kJ/mol. For the corresponding possibilities of hydrogen bonded complexes [silicon dioxide---$(H_2O)_n$] this value is -20 kJ/mol. When the solvent effect is considered, the $\Delta_r H$ PM7 of [(calcium hydroxide)---$(H_2O)_n$] hydrogen bonded complexes, in average, is -17 kJ/mol, where the corresponding value of [(silicon dioxide)---$(H_2O)_n$] hydrogen bonded

complexes is only -5 kJ/mol. In conclusion, being the calcium hydroxide the mainly component of plastering mortar, the enthalpy of the formation of hydrogen bonds, as well as the water effect in this property, seemingly, are associated with the mechanical behavior of tensile strength of this mortar when applied in the facades of structural masonry buildings.

Key-words: hydrogen bonds; semiempirical; mortar; roughcast; tensile strength.
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